MECHANISM OF ELECTROSTRICTION — A FEASIBILITY STUDY

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To complete the picture of the microscopic processes of electrostriction obtained by synchrotron radiation measurements a complementary neutron diffraction experiment is planed. The promising results of a first test measurement reported here show which improvements in the set up have to be made.

The explanation for the piezo electric effect (deformation of a crystal in an electric field) given in most textbooks is based on *polarization densities*. Besides for molecular crystals, polarization in a crystal is not well defined and depends on the choice of the unit cell. A consistent theoretical description of a crystal in a non-vanishing external electric field is still not possible [1].
The deformation ε of a crystal caused by an external electric field $\mathbf{E}$ is described by the tensor of (first order) electrostriction $\mathbf{d}$ with $\varepsilon = \mathbf{dE}$. This macroscopic effect can be reduced to a change of the unit cell parameters. The quantity $\mathbf{d}$ contains no information about the processes within the unit cell as changes of bond lengths and angles or ionic charges.
The microscopic response of a series of crystals to a homogeneous external electric field was measured in the past to supply experimental data for the comparison with theoretical models and calculations [2]. The measured quantity was the intensity R of a Bragg reflection as a function of E. These measurements were performed at the synchrotron radiation sources HASYLAB and ESRF [2,3].
The relative intensity variation $(\Delta R/R_0)(E)$ for some measurements is non-linear for small E, as shown in Fig. **1**. Synchrotron radiation probes the charge density and is (in this case) reflected in a volume close to the surface so that charge accumulation close to the electrodes may lead to the observed non-linearity.

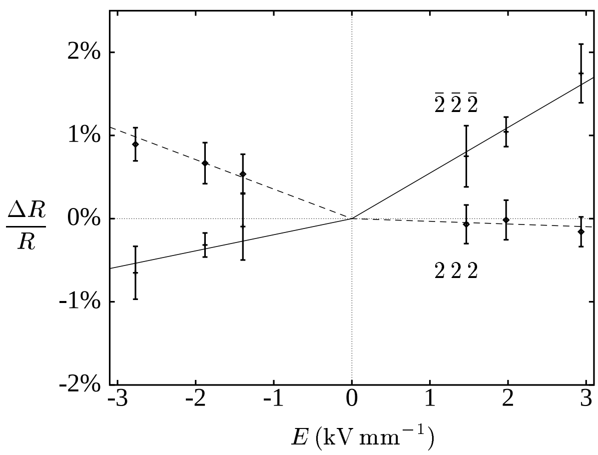

Fig.1: Relative intensity variation for the reflections $2\,2\,2$ and $\bar{2}\,\bar{2}\,\bar{2}$ of GaAs as functions of the electric field strength. The measurements were performed with synchrotron radiation at the 4 axes spectrometer at HASYLAB.

The complementary experiment with neutrons allows to clear up this point because there only the nuclei contribute to the intensity and the whole crystal is probed, which is a guaranty that bulk properties are measured.
To find out if such an experiment with neutrons will be successful, a first measurement was performed on the 2 axes neutron spectrometer TOPSI at SINQ. The sample was a $1\,1\,1$ oriented GaAs single crystal waver (thickness $0.5\,\mathrm{mm}$) which was coated with silver layers on both sides to form a plate capacitor like structure. The DC-voltage is supplied via a shielded cable from the electronics rack to a socket close to the sample and from there via thin copper wires to the silver electrodes. The capacity of the long shielded cable prohibited a fast switching between the states $E = 0$ and $E \neq 0$ which made a measuring regime impossible as used in the former experiments [3].
To get sufficient statistics, the measure time per ω value and voltage was about $20\,\mathrm{s}$; For each of the 81 ω positions both states were measured only once; The sacn was repeated 10 times.
The measured mean intensity variation for GaAs $\bar{2}\,\bar{2}\,\bar{2}$, $E = 1\,\mathrm{kVmm^{-1}}$ is $\approx 0.9\,\%$. The accuracy for the individual rocking curves calculated using Poisson statistics only is $6\cdot 10^{-4}$. In contrast to this the variance of the single experiments is a factor of 5 larger. This means that there are some unwanted influences leading to time dependent systematic errors. Since the sample was unshielded against the environment, temperature variation and visible light irradiation could affect the resistance and thus the current through the sample. Indeed the current varied between $5\,\mu\mathrm{A}$ and $80\,\mu\mathrm{A}$ from one ω value to the next.
The measurements performed at night are much closer to the mean value compared to those performed at daytime. This supports the need for more stable conditions for further investigations.

The detection of small dislocations of atoms due to an external electric field with neutron diffraction is possible if a lot of effort is spent in the reduction of environmental influences and on the sample preparation.

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[1] R. Resta, Rev. Mod. Phys. **66**, 899-915 (1994)
[2] J. Stahn, U. Pietsch, P. Blaha and K. Schwarz, Phys. Rev. B **63**, 165205 (2001)
[3] J. Stahn, A. Pucher, T. Geue, A. Daniel and U. Pietsch, Europhys. Lett. **44**, 714 (1998)